# CHBE 590

# KINETICS, CATALYSIS, AND REACTION ENGINEERING

# Fall 2017

## Instructor

Kyriacos Zygourakis, Abercrombie B227, kyzy@rice.edu
Lectures: TR 1:00 - 2:15 PM - GRB W212
Office Hours: TR 4:30 - 5:30 PM

## Course Contents

1. **Introduction**.
2. **Stoichiometry**: Independent reactions; reaction and production rates; computational aspects.
3. **Thermodynamics**: Reaction heat effects and chemical equilibrium.
4. **Material Balances for Chemical Reactors**: General equation for conservation of mass; batch, semi-batch, continuous stirred tank (CSTR) and plug flow reactors.
5. **Chemical Kinetics**: The reaction equilibrium and quasi-steady state assumptions.
6. **Energy Balances for Chemical Reactors**: Well-mixed reactors, CSTR steady-state multiplicity and limit cycles. Empty tube flow reactors, hot spots and runaways.
7. **Diffusion and reaction in catalyst pellets**: Effectiveness factors for isothermal and non-isothermal catalyst pellets, external mass transfer, reactions with Langmuir-Hinshelwood kinetics.
8. **Design of fixed-bed catalytic reactors**: Convection, dispersion and external mass transfer; 1D and 2D pseudo-homogeneous and heterogeneous models.

## Textbook

J.B. Rawlings and J.G Eckerdt, “Chemical Reactor Analysis and Design.” Second Edition, Nob Hill Publishing (2013).

## Homework Assignments

Homework problem sets will involve both theoretical analysis and computer programing. Students should use MATLAB for the solution of homework problems. A few recitation

sessions will be held in the beginning of the semester to remind students how to use MATLAB to solve nonlinear systems of equations and integrate systems of differential equations.

**Homework Policy**

- Late homework will be penalized, unless prior permission has been obtained from the instructor.
- Homework that is more than two days late will not be accepted.
- Late homework will not be accepted after solutions have been posted.

**Exams**

There will be a midterm exam on October 12 and a second exam during the week of finals (12/6 to 12/13).

**Grading Policy**

- Homework: 40%
- Exams: 60% (25% and 35%)

The raw scores earned for the homework and exams will be converted to t-scores. The final course grade will be assigned using the weighted averages of all the t-scores.

**Honor Code Policy**

Students may talk to each other, the course TA(s), and the instructor about any assignment in the course that is not specifically designated as pledged. This assistance is limited to a discussion about the fundamental concepts involved in solving the problem. Students are not allowed to share calculation details and computer codes, or to consult another student's solution (even from a previous CHBE 590 or another reaction engineering class). Submitted solutions to assignments may not be copied from any source

**ADA Statement**

Any student with a documented disability needing academic adjustments or accommodations is requested to speak with the instructor during the first two weeks of class. All discussions will remain confidential. Students with disabilities will need to also contact Disability Support Services in the Ley Student Center.